Particle with internal dynamical asymmetry: chaotic self-propulsion and turning

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Abstract

We consider model of a complex particle that consists of a rigid shell and a nucleus with spatial asymmetric interaction. The particle's dynamics with the nucleus driven by a periodic excitation is considered. It is shown that unidirectional self-propulsed particle motion arises in the absence of spatial and temporary asymmetry of external potentials and influences. Transport modes are the general case of complex particle dynamics in the presence of nonlinear friction or periodic external potential. The changes of average transport velocity and direction of transport are determined by qualitative changes of internal dynamics regimes: local attractor bifurcations in the internal phase space of the complex particle. Finally, microbiological relevance of the proposed model is briefly discussed.

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Over the past years, the appearance and intensive development of some areas of nonlinear dynamics and statistical physics have been inspired by several microbiological phenomena [1-4]. First, it is the physical principles and functional mechanisms of molecular motors, nano- and microscale engines, which effectively convert chemical energy to mechanical work [1]. Second, it is physics of motility, namely the unidirectional transport of microbiological objects [2]. Both these research lines are closely related to each other, and the biological motor efficiency can be defined in the terms of average transport velocity[3].

One of the most interesting mechanisms of the directed transport of microobjects is the so-called ratchet-effect, related to particle motion in periodic potential with spatial asymmetry [4]. As a rule, the problem of the ratchet mechanism is considered within the frame of stochastic approach, when the unidirectional motion of overdamped Brownian particle in asymmetrical potential takes places due to unbiased nonequilibrium fluctuations in the absence of any macroscopic forces and gradients [4-5]. However, recently a significant interest has been paid to the deterministic approach to this problem, taking into account the finiteness of inertial terms [6-7]. A deterministic description allows to expand dynamic modes spectrum, including regular and chaotic ones [8], and to study the role of interaction mechanisms in greater detail. Within the framework of this approach, similar to the deterministic diffusion phenomenon [9], low-dimensional dynamic chaos can effectively play the role of thermodynamic fluctuations. In [7], Mateos studied the event of the deterministic motion of a particle in smooth ratchet potential under the action of a symmetrical periodic time-dependent force. He showed that a wide spectrum of dynamic regimes, with bifurcation transitions between regular and chaotic regimes, arises when periodic force amplitude is varied. Moreover, he found, that current reversals are related with bifurcations from chaotic to periodic regimes. In a recent paper [10], Flach, Yevtushenko and Zolotaryuk have studied a more general case of a directed current appearance in deterministic nonlinear systems. It has been shown that the key factor for a transport regime appearance is the existence of spatial ("spatial ratchet") and/or temporary ("temporal ratchet") asymmetry of influences upon a particle.

Thus, one of the necessary triggers for directed transport appearance is the existence of asymmetry in the system. The basic idea of the present paper is that this asymmetry can be "built" into the internal degrees of freedom of the complex particle and, in this way, the source of motion can be located inside of the object itself. At that, external potentials and the influences can be completely symmetrical [11]. Such a particle is an active self-propulsed walker, which can control the direction and velocity of its own motion. Further we will formulate a simple one-dimensional model of a complex particle and we will consider its dynamics in: (i) a medium with nonlinear friction (that is true for real biological media nearly always [12]) and (ii) in a linear medium under external periodic symmetrical potential. We will analyse spectrum of dynamic regimes that arises under changing parameters of the system, and also the relations between the peculiarities of a complex particle internal dynamics and its directed transport characteristics. Finally, we will shortly discuss the biological motivation of the proposed model.

Let us consider a one-dimensional system, consisting of a rigid spherical shell with a mass M, whose position is determined by the coordinate of its centre X, and an internal particle ("nucleus") with a mass m and the coordinate x, attached to the internal walls of the shell (see inset in Fig1.). The elastic interaction between the shell and the nucleus is governed by an asymmetric nonlinear potential $U(x - X)$, so that the force arising due to the nucleus displacement from the centre of the shell depends not only on the absolute

displacement value $\Delta x = x - X$, but also on its sign (Fig.1). The minimum of the potential is located at the origin ($U^{'}(x) = 0$), which corresponds to the equilibrium nucleus position in the centre of the shell. Let us also presume that the nucleus is driven by a periodic symmetrical force $f(t) = acos(\omega t)$ which is defined, for example, by mechanochemical coupling to a periodic biochemical reaction, such as ATP hydrolisis [13]. Then, generally, with an external potential and nonlinear friction present, the complex particle dynamics, after trivial mass normalisation, is defined by the pair of equations:

$$\ddot{x} = -K_1(\dot{x} - \dot{X}) - \frac{\partial U(x - X)}{\partial x} + acos(\omega t), \quad (1)$$

$$\ddot{X} = -K_2(\dot{X}) + \mu \frac{\partial U(x - X)}{\partial x} + W^{'}(X) \quad (2)$$

where $K_i(\nu)$ are nonlinear friction forces, $\mu = \frac{m}{M}$ is the mass factor, a, ω are driving force amplitude and frequency respectively. The potential of interaction is given by (Fig.1):

$$U(x) = \alpha(x - x_0)^2 + \beta(x - x_0)^4 - \gamma(x - x_0)^3 \quad (3)$$

where α, β, γ are the parameters of interaction, x_0 is an appropriate shift, such that a minimum of potential (3) is located at the origin. Nonlinear friction forces are given by $K_i = s_i\nu + q_i\nu^3$. The parameters $\mu = 2, \omega = 1, \alpha = \beta = 1, \gamma = 2.5, x_0 \approx 1.553$ are fixed throughout this paper.

The complete phase space of the system (1-2) is five-dimensional $(x, X, \dot{x}, \dot{X}, t)$, the dynamic equations are nonlinear and contain dissipative terms. So, in the phase space of system (1-2) both periodic (limiting cycles) and chaotic (strange attractors) attractors can exist [8]. On the other hand, the complex particle structure induce, in the natural way, the splitting of the complete phase space into two subspaces, the external one, accessible to an external observer - $(X, \dot{X}, t)$, and the internal one, corresponding to an observer located within the shell - $(x - X, \dot{x} - \dot{X}, t)$. The first subspace corresponds to nonlocal transport of the complex particle as a whole, the second one corresponds to local dynamics, which is determined by the internal interaction. The most interesting question is how the correlation between these two scales of the particle's complete dynamic is realised. While zero-mean driving symmetrical periodic force $f(t)$ does not contain a constant component, the appearance of the directed current can only be a consequence of the asymmetry of the internal interaction.

Let us consider now the motion of a particle in a nonlinear medium in the absence of an external potential ($W(x) \equiv 0, s_1 = 0.2, s_2 = 0.5, q_1 = 10^{-2}, q_2 = 5 \cdot 10^{-3}$). For the analysis of the particle's dynamics in the external phase space $(X, \dot{X}, t)$ we used stroboscopic Poincare section [8] with the period equal to the driving force period, $T = 2\pi/\omega$. The bifurcation diagram for $V = \dot{X}$ in a limited range of the parameter a is shown in Fig.2a [14]. At first, the standard scenario of period-doubling route to chaos is realised ($a \in [5.6, 6.0347]$), and then the bifurcation connected with the internal crisis of a chaotic attractor ($a_1 \approx 6.2117$) and the opposite tangent bifurcation connected with the birth of a steady period-three cycle take place ($a_2 \approx 6.96441$) [8]. In Fig.2b we show the current $J = \frac{1}{NM}\sum_{j=1}^{M}\int_{t_0}^{t_0+N} V_j(t)dt$, ($t_0 = 50, N = 10^4, M = 50$), as the function of parameter a in the same range of values. As one can see, current reversal takes place exactly at the tangent bifurcation point a_2. As viewed from the internal phase space $(x - X, \dot{x} - \dot{X}, t)$ it

corresponds to transition from the chaotic attractor (Fig.3a) to the periodic one (Fig.3b). Besides, a smaller jump of the current value takes place at the internal crisis bifurcation point a_1, that corresponds to a sudden expansion of chaotic attractor [15]. It can be shown that by a certain variation of the system parameters it is possible to achieve the current reversal taking place exactly at this bifurcation point. The investigation of the model's dynamics in other ranges of parameter a showed, that any abrupt change of the current J is connected with sudden changes of the internal chaotic attractor - *crisis* (as interior crisis at a_1), or *subduction* (as tangent bifurcation at a_2) [15]. Here, current reversal with the a greater probability occurs at bifurcations of the second type, that is tangent bifurcations (as in this case the jump of a current value is much greater).

Let us consider now the motion of a complex particle under external periodic potential $W(x) = Acos(X)$. To separate nonlinear friction mechanisms, let us presume that the medium is linear ($q_i \equiv 0$). We found that in this case, as well as in the one considered above, there also exist transport modes. However, unlike the free motion case, in this case the transport modes take place within certain parameter ranges. It is connected with the presence of external potential, which adds to the system some additional temporal and spatial characteristic scales, while some coherence between the parameters of external potential and internal force and interaction is needed for the appearance of transport. We found a very interesting effect which is connected with these coherence mechanism, the effect of sharp change (current "switching") (Fig.4b). In the parameter space this effect looks like full overbarrier reflection, when the particle flying in the ballistic mode above potential ($V_m = \int_0^T V(t)dt = 1, a \in [5.1, 5.206]$) changes its flight direction to the opposite ($V_m = \int_0^T V(t)dt = -1, a \in [5.363, 5.57]$) at a small variation of the driving force amplitude. The corresponding bifurcation diagram for V is shown in Fig.4a. As one can see, the current switching, as it is in the nonlinear friction case, is connected with tangent bifurcation at $a_c \approx 5.3633$ leading to the birth of the limiting cycle from the chaotic attractor. The period-one limiting cycle of the particle internal phase space C_1 corresponds to the ballistic transport in the positive direction in the region, while another period-one cycle, C_2, corresponds to the transport in the negative direction (see inset in Fig.4a).

The existence of these limiting cycles, C_1 and C_2, allows to distinguish between two characteristic spatial scales and to separate the solution in the external phase space into two parts $X(t) = X_s(t) + \xi(t)$, where $X_s(t)$ is a slow part and $\xi(t)$ is a small fast part. After that, using perturbation theory ideology [16], for the slow variable we can construct a "quasi" zero-order approximation:

$$\ddot{X}_s = -s_2 X_s + W'(X_s) + S(t) \tag{4}$$

where

$$S(t) = G(x(t) - X(t)) = \frac{\partial U(x(t) - X(t))}{\partial x(t)} \tag{5}$$

is a periodic force acting on the shell that corresponds to the exact solution of the system (1-2). This forces $S(t)$ is zero-mean, $\int_0^T S(t)dt = 0$, with pronounced temporal asymmetry (Fig.5a and Fig.6a). Thus, the equation (4) describes the motion of a *simple* particle under a periodic potential, driving by a spatially homogeneous *asymmetric* periodic force [10]. For the numerical integration of the equation (4) we used as excitation force the

first six harmonics of the complete solution, $S^{*}(t)=\sum_{k=1}^{6} S_k cos(k\omega t+\phi_k)$. The obtained results demonstrate very close agreement with the solutions of the entire system (1-2). In C_1 - case in the in phase space of system (4) there exists the only one global attractor that corresponds to the particle ballistic transport in the positive direction (Fig.5a), and in C_2 - case there is the only one global attractor that corresponds to the particle ballistic transport in the negative direction (Fig.5b). In the case of chaotic transport (e. g., $a \in [2.208, 5.363]$) approximation (4) is not valid, because due to spectrum continuity there are no distinguished scales in the system.

It is necessary to note, that in each of the considered cases (free motion in nonlinear medium and motion under external periodic potential), there is only one global attractor (limit cycle or chaotic attractor) in the phase space of system (1-2) for the given value of parameter a. In those cases averaging over ensemble is equivalent to averaging over attractor invariant measure, and so we can talk about the directed motion of an individual self-propulsed complex particle rather than of current. The obtained current J dependencies can be represented as dependencies of the average drift velocity V_m of the particle, and we also can talk about turning instead of current reversal.

In summary, we have shown, that the internal dynamic asymmetry, "dynamical chirality ", can be a source of the directed motion of a complex particle. Transport modes are not exceptional, but occupy certain parameter ranges (it is a general case for the motion in a nonlinear medium). The direction and velocity of the motion are determined by the particle internal dynamics properties, and their changes are connected with the internal attractor bifurcations. It is interesting to note, that a similar situation will take place, if we consider a particle with symmetrical nonlinear internal interaction $U(x)$ and a temporal asymmetrical driving periodic force $f(t)$ [17]. Such a force may be stimulated by a limiting cycle of some biochemical reaction [18], which is conformally coupled with the internal particle structure. Here, the force temporal asymmetry will be a general case, while symmetry is possible as an exceptional case in the space of reaction parameters.

The assumption of absolute rigidity of the shell is not a strict requirement. The validity of such assumption corresponds to the validity of the inequality $\theta = \omega_s/\omega \ll 1$, where ω is the driving force frequency and ω_s is the characteristic frequency of large-scale deformation vibrations of the shell. Moreover, the viscosity of the external and internal medium also impedes the excitation of such oscillations. The energy dissipation by the small shell vibrations can be taken into account within nonlinear friction terms.

The considered mechanism can shed light upon physics of some non-canonical forms of microbiological motility. For example, swimming Cyanobacteria, having the shape of almost exact spheroid and having no external appendages perform directed motion in a liquid without any observable shape changes [19]. The mechanism of internal dynamic asymmetry can be additional to the hydrodynamic mechanism accounting for the transport of Cyanobacteria through to small-scale periodic modulations of the shell shape [20]. In the case of more complex cells, the internal structure of the particle can be a concentrated image of the cytoskeletal structure [13]. Cytoskeletal polymers all have complex nonlinear viscoelastic characteristics [21]. Moreover, interactions between cytoskeletal polymer systems in living cell may result in composite material with unique nontrivial dynamic properties [22]. Furthermore, the proposed model provides for dynamic modelling of such collective phenomena, as microorganisms interaction and self-organisation at the level of microscopic equations of the motion of a single biological particle. The microscopic approach to these phenomena that consider a microorganism as an active object

in active environment [23], makes it possible to effectively use the ideas about interaction and synchronization of internal attractors of individual microobjects [24].

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FIGURE CAPTIONS

1. The interaction potential $U(x)$ between shell and nucleus. Inset shows the complex particle structure.

2. (a) Bifurcation diagram for V as a function of a and (b) the current J as a function a for $\mu = 2, \omega = 1, \alpha = \beta = 1, \gamma = 2.5, W(X) \equiv 0, s_1 = 0.2, s_2 = 0.5, q_1 = 10^{-2}, q_2 = 5 \cdot 10^{-3}$.

3. Projections of complex particle internal phase space attractors: (a) chaotic attractor for $a = 6.96$ and (b) the period-three limit cycle just below tangent bifurcation at $a \approx 6.9644$.

4. (a) Bifurcation diagram for V as a function of a and (b) the current J as a function a for $A = 3, s_1 = 0.5, s_2 = 0.8, q_1 = q_2 \equiv 0$. Inset shows (a) internal phase space period-one limit cycles: C_1 ($a = 5.18$, positive current) and C_2 ($a = 5.41$, negative current) and (b) corresponding particle trajectories.

5. (a) The shape of periodic zero-mean asymmetric force $S(t)$, corresponding to limit cycle C_1 ($a = 5.18$, positive current): solid curve - exact solution for system (1 - 2), dotted curve - first six harmonics sum; (b) corresponding limit cycle in the reduced external phase space ($V_m = 1$): solid curve for full system (1), dotted curve - for approximation (4) with the first six harmonics as driving force.

6. Same as in Fig.5 for cycle C_2 ($a = 5.41$, negative current).

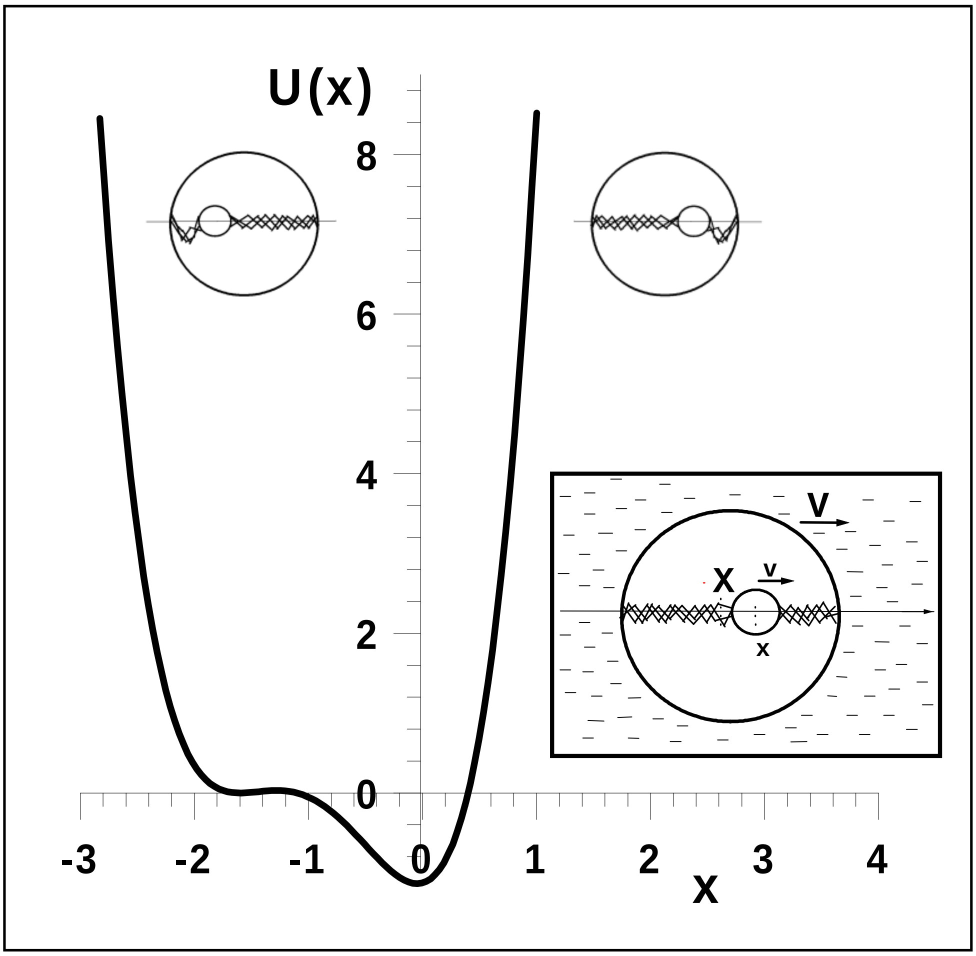


FIG. 1

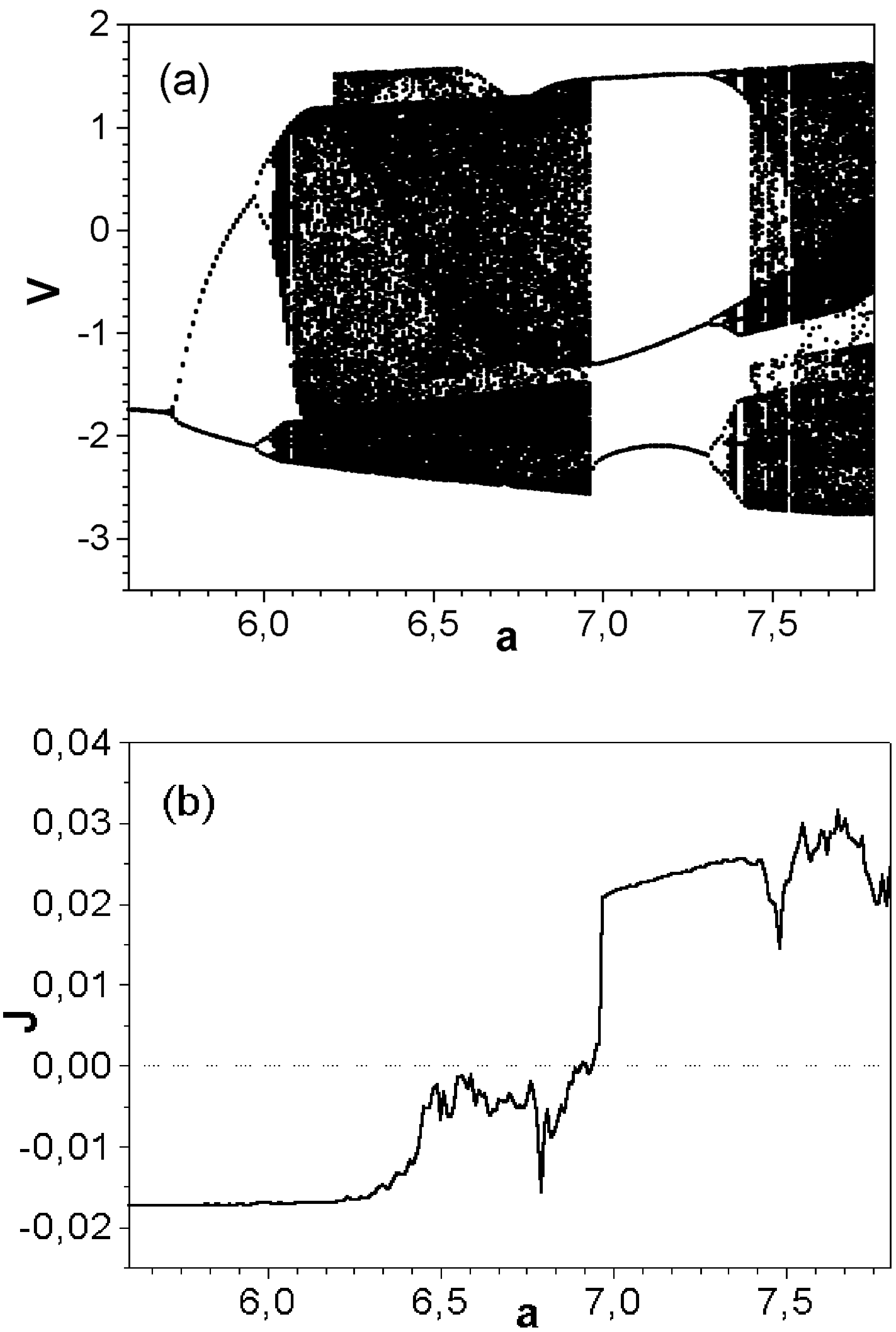


FIG. 2

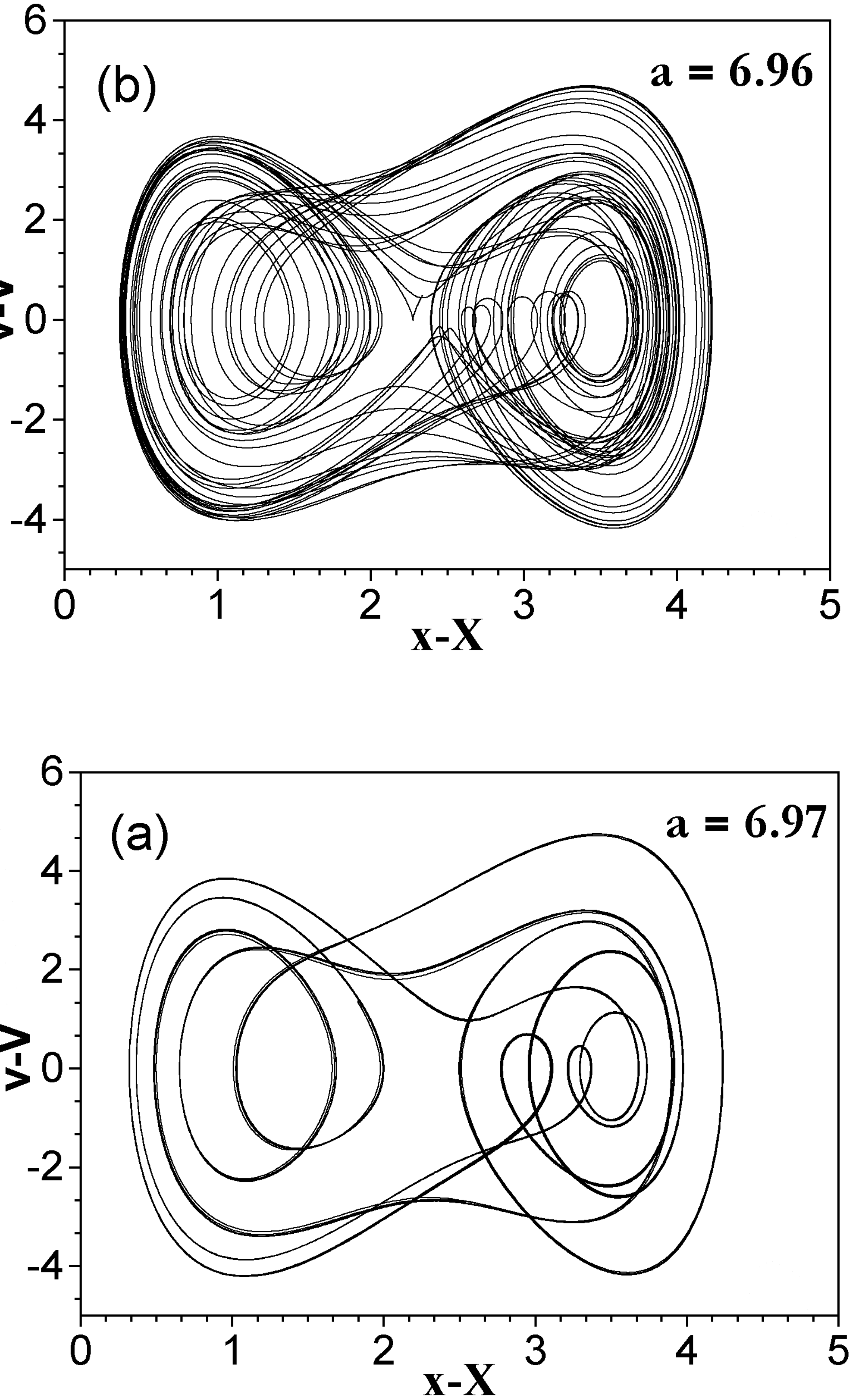


FIG. 3

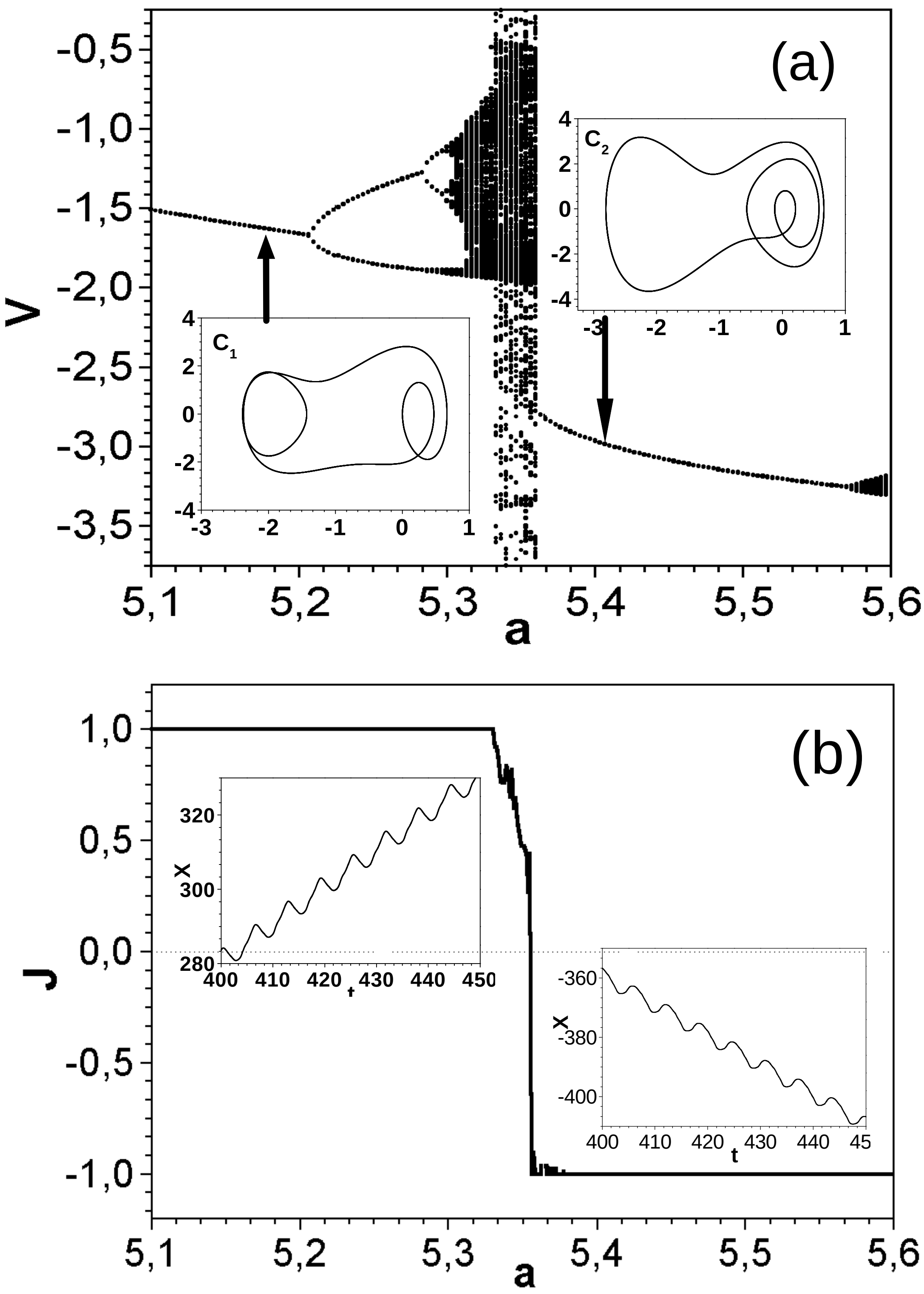
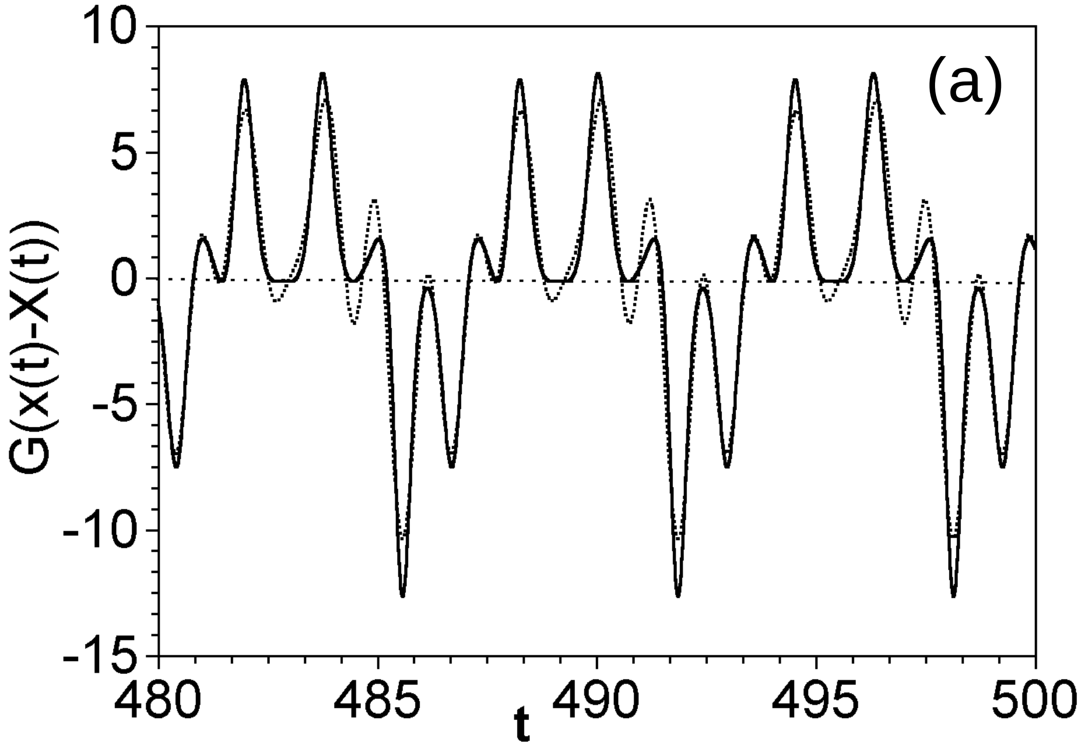
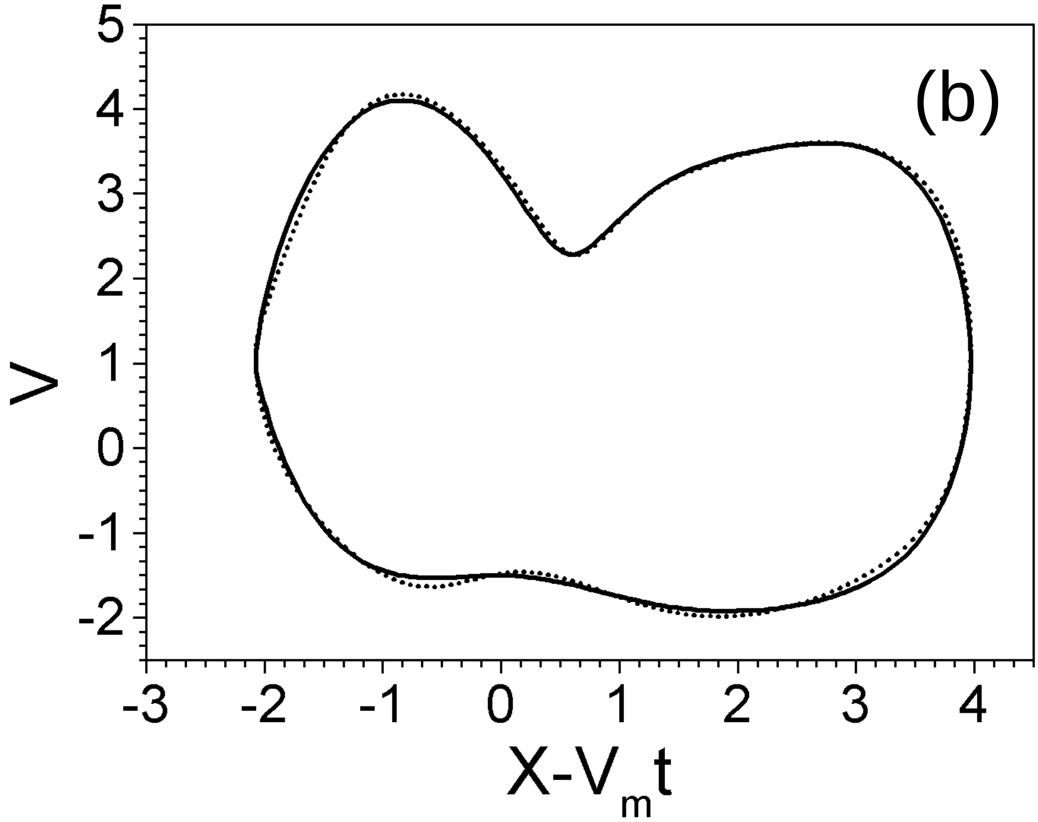


FIG. 4



(a)
G(x(t)-X(t))
10
5
0
-5
-10
-15
480
485
490
495
500
t



(b)
V
5
4
3
2
1
0
-1
-2
-3
-2
-1
0
1
2
3
4
X-V$_m$t

FIG. 5

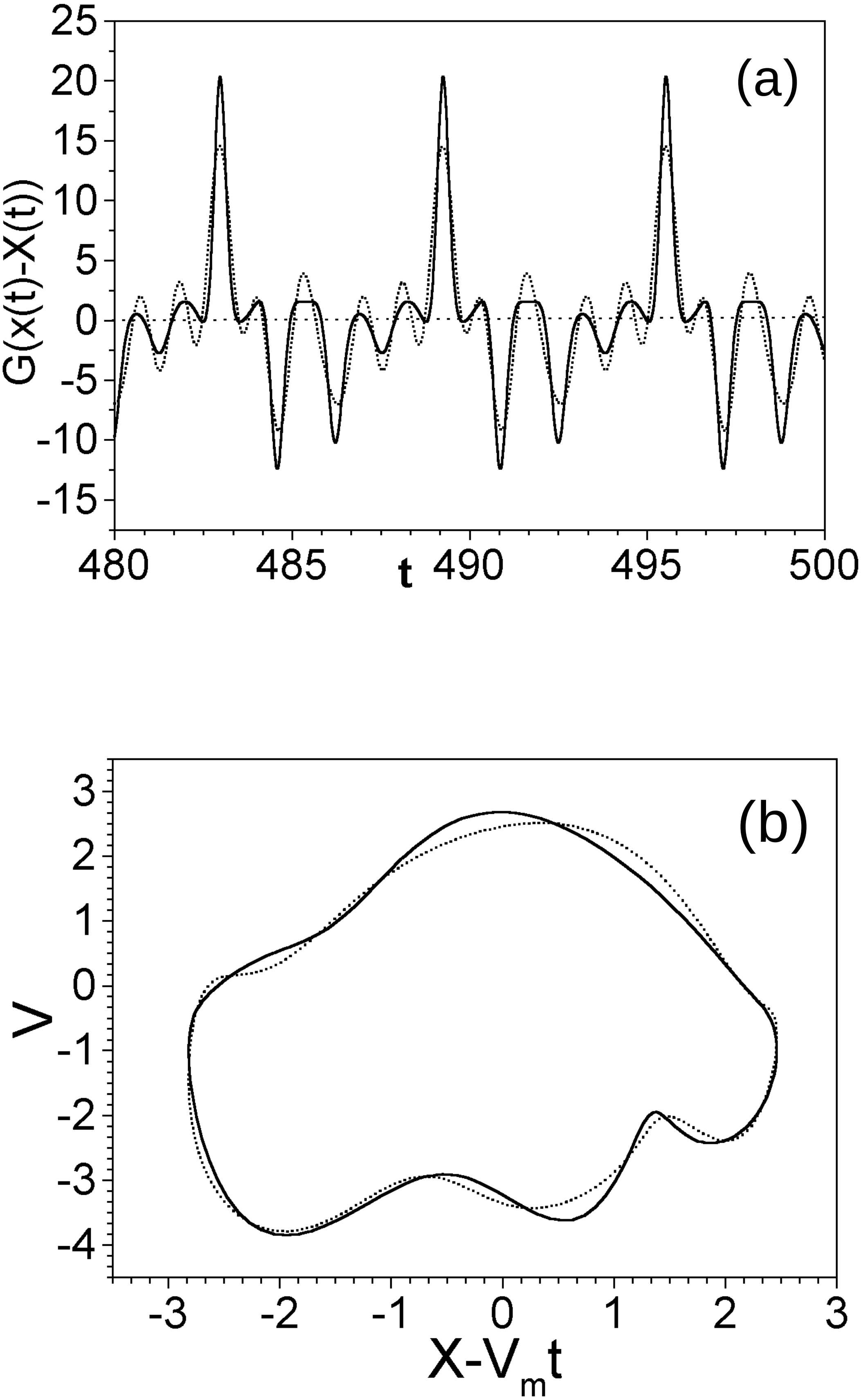

(a)
G(x(t)-X(t))
t
25
20
15
10
5
0
-5
-10
-15
480
485
490
495
500
(b)
V
X-V_m t
3
2
1
0
-1
-2
-3
-4
-3
-2
-1
0
1
2
3

FIG. 6